Analyzing and Communicating Scientific Data with Visual Analytics

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I guess I don't need to tell NASA we live in the "Data Era" right? :)

We all understand data has lots of value ...

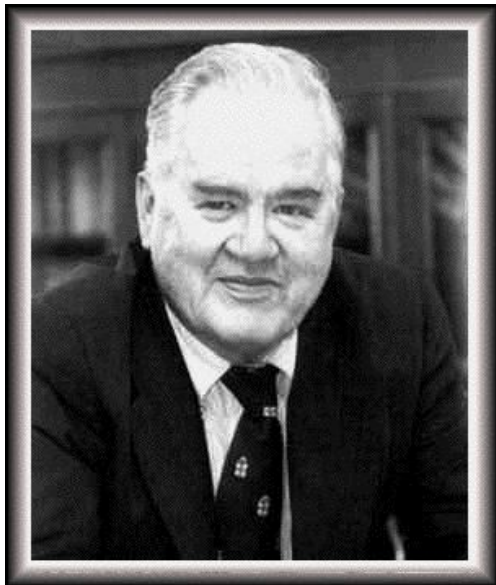… but how do we extract useful information and knowledge out of data?

… and how do we communicate this information *effectively*, *truthfully*, and *persuasively* to others?

Traditional scientific process:

1) Formulate a question first.
2) Collect necessary data.
3) Run experiment to answer the question.

… when data largely available/easy to produce:

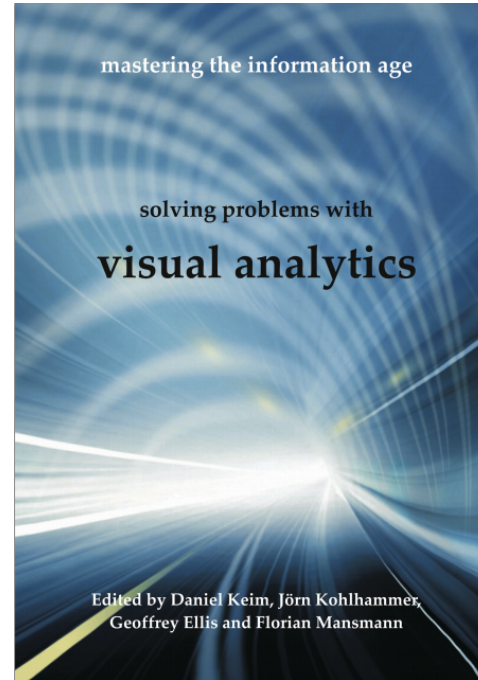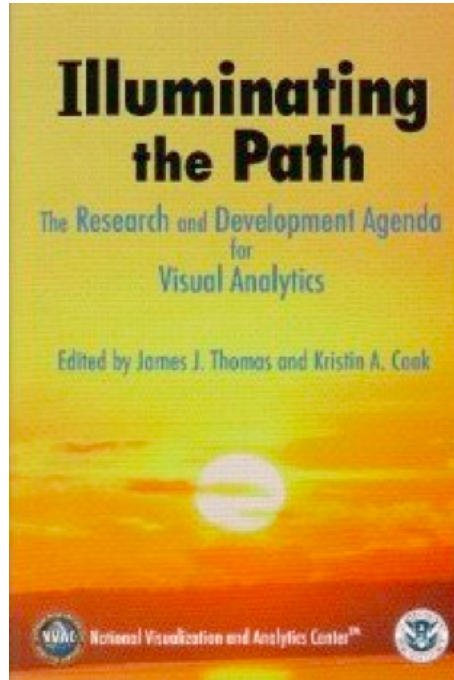1) We got data! What shall we do with it?
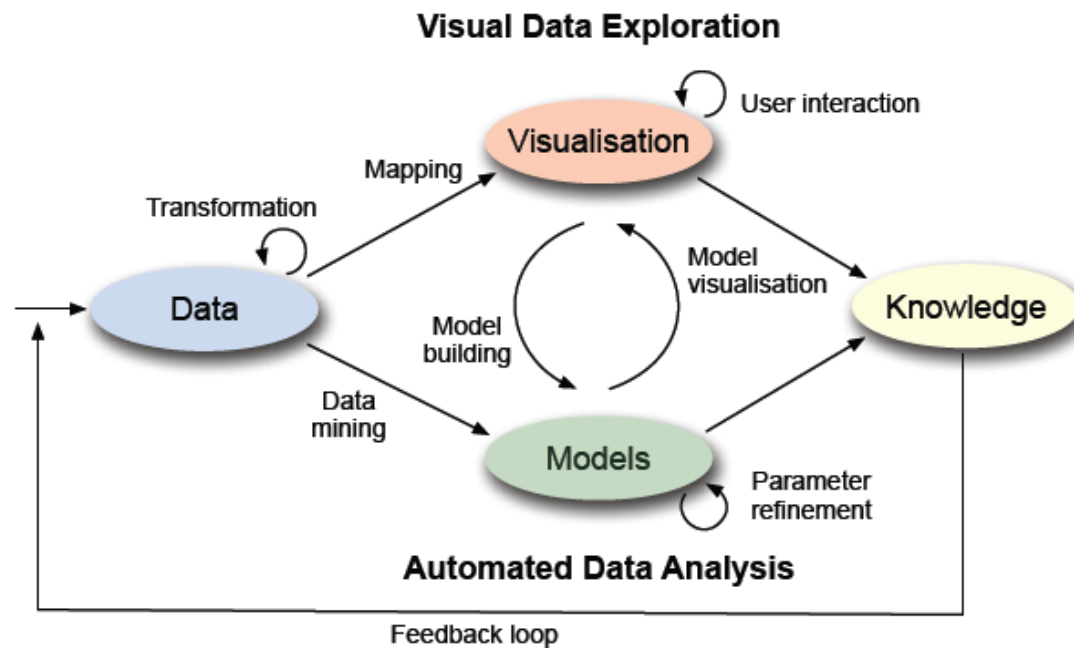2) Let's look into it.
3) Mmm … How?

JOHN W. TUKEY*

We often forget how science and engineering function. Ideas come from previous exploration more often than from lightning strokes. Important questions can demand the most careful planning for confirmatory analysis. Broad general inquiries are also important. Finding the question is often more important than finding the answer. Exploratory data analysis is an attitude, a flexibility, and a reliance on display, NOT a bundle of techniques, and should be so taught. Confirmatory data analysis, by contrast, is easier to teach and easier to computerize. We need to teach both; to think about science and engineering more broadly; to be prepared to randomize and avoid multiplicity.

Visual Analytics: "The science of analytical reasoning facilitated by interactive visual interfaces"

Visual Data Exploration

Visual Data Exploration

Visualisation — User interaction

Mapping

Transformation

Data

Data mining

Model building

Model visualisation

Models

Knowledge

Parameter refinement

Automated Data Analysis

Feedback loop

Examples from our lab ...
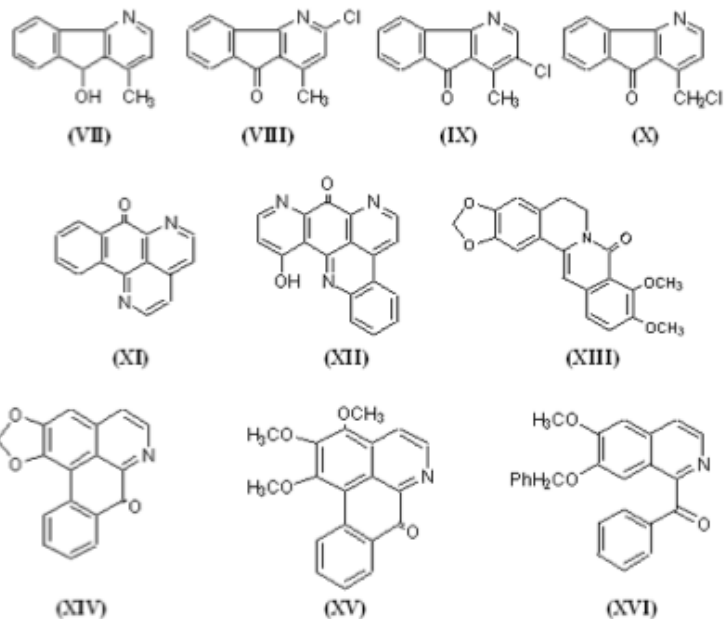
a. Visual Analytics for Drug Discovery.

Assay Plates

Negativ **Positiv** Neçativ Negativ **Positiv** Negativ Negativ

Plate Reader

SYNERGY

Data

Structure-Activity Relationship (SAR) Analysis

(VII) (VIII) (IX) (X) (XI) (XII) (XIII) (XIV) (XV) (XVI)

	O-S-C (=O)	S-C-N (=O)	S-C-N (-C)	S-C-N	C-N-C
O-S-C-N (=O)	1	1	0	1	0
S-C-N-C (=O)	0	1	1	1	1

Mining algorithms necessary to extract meaningful molecular fragments.

HiTSEE

Bertini, Enrico, et al. **"HiTSEE: a visualization tool for hit selection and analysis in high-throughput screening experiments."** Biological Data Visualization (BioVis), 2011 IEEE Symposium on. IEEE, 2011.

b. Visual Comparison of Machine Learning Models for Healthcare Analytics.

Predictive Modeling Pipeline

Running Example: Predicting Diabetes Diagnoses in a Patient Population

Cohort Construction	Feature Construction	Cross Validation	Feature Selection	Classification
Constructs a cohort of 15,038 patients. 50% (7,519) have a diabetes diagnosis	Assembles a feature vector using 4 types of clinical events: Diagnoses, Labs, Medications, and Procedures	Splits the cohort into 10 random folds for Cross Validation	Executes 4 Feature Selection algorithms on each fold: Information Gain, Fisher Score, Odds Ratio, and Relative Risk	Evaluates each model of selected features with 4 classifiers: Logistic Regression, Decision Tree, Naïve Bayesian, and K Nearest Neighbor

(Work in collaboration with Adam Perer @ IBM Watson)

Parallel computation of multiple models

Feature Selection
(Information Gain, Fisher Score,
Odds Ratio, Relative Risk, …)

X

Classification
(Logistic Regression, Decision
Trees, Naive Bayes, kNN, …)

X

Folds (Samples)
10-folds validation

INFUSE

- Each dot is a feature (e.g., lab test)

- Each quadrant represents a feature selection algorithm

- Each segment represents a fold (sample)

- Length of the bar represents the ranking

DIAGNOSIS - HCC
DIAGNOSIS - ProblemList
Lab - Lab
Medication - Ingredient
Medication - Orders
PROCEDURE - Cpt code

Information Gain
Fisher Score
Odds Ratio
Relative Risk

c. Visual Reconciliation of Alternate Similarity Spaces in Climate Modeling.

Model Structure

criteria

models

Create groups

Reconcile structure with output

Reflect → Split

Optimize ← Reflect

Reconcile output with structure

Model Output

models

time

Create groups

Initial state

(a)

(e)

Reflect

Reflect

Iterative Analysis

(b)

(d)

(c)

Optimize weights

Select criteria to create groups

North American Temperate

(d)

(e)

(f)

Why use visualization?

Visualization can make complex problems trivial.

Let's Play a Game! The Game of "15"

RULES

1) There are 2 players

2) Each player takes a digit in turn

3) Once a digit is taken, it cannot be used by any of the players again

4) The first player to get three digits that sum to 15 wins

{1, 2, 3, 4, 5, 6, 7, 8, 9}

Tic-Tac-Toe: Herbert Simon's "Problem Isomorph"

4	9	2
3	5	7
8	1	6

Visualization can be faster than your eyes can move!

Preattentive Processing

Preattentive features can be detected faster than eye movement (200 msec).

Visualization can reveal information that summary statistics may hide.

Anscombe's Quartet

Property	Value
Mean of x in each case	9 (exact)
Variance of x in each case	11 (exact)
Mean of y in each case	7.50 (to 2 decimal places)
Variance of y in each case	4.122 or 4.127 (to 3 decimal places)
Correlation between x and y in each case	0.816 (to 3 decimal places)
Linear regression line in each case	$y = 3.00 + 0.500x$ (to 2 and 3 decimal places, respectively)

But … only if used properly!

Example taken from: Junk Charts: Expanding circles of error
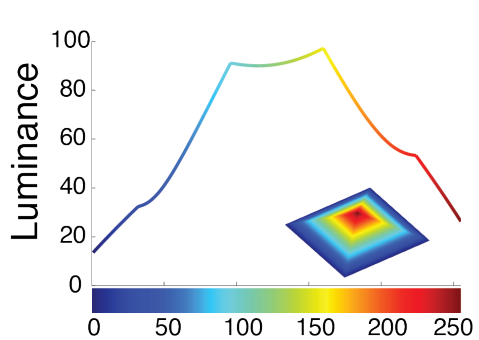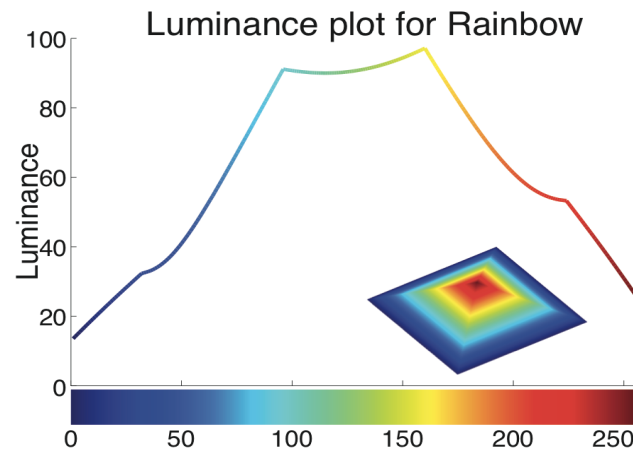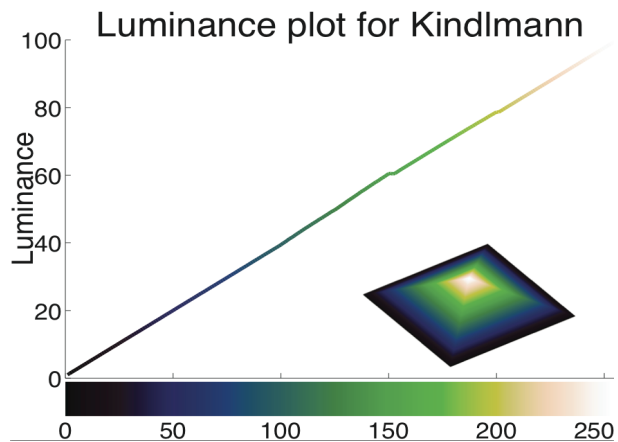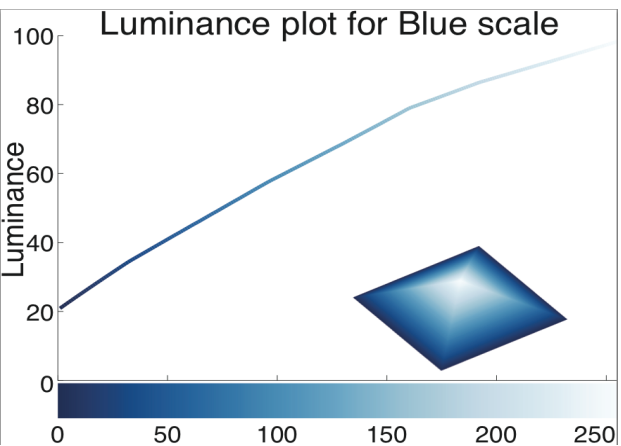
Some are plain wrong!

Graphical Perception

Cleveland, William S., and Robert McGill. "Graphical perception: Theory, experimentation, and application to the development of graphical methods."*Journal of the American Statistical Association* 79.387 (1984): 531-554.

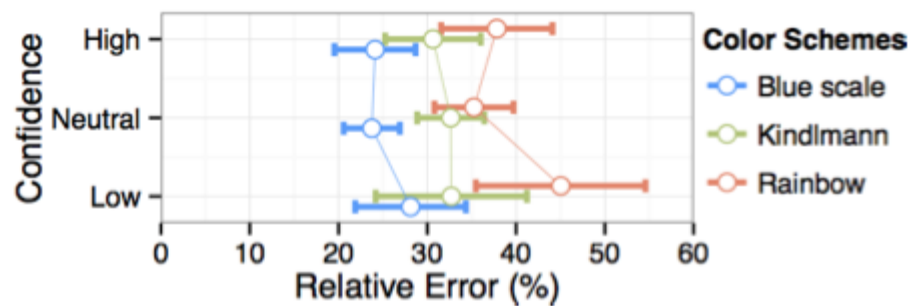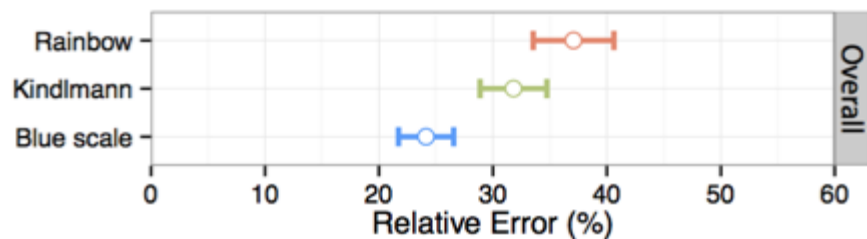# Evaluation of Color Maps in Climate Science.
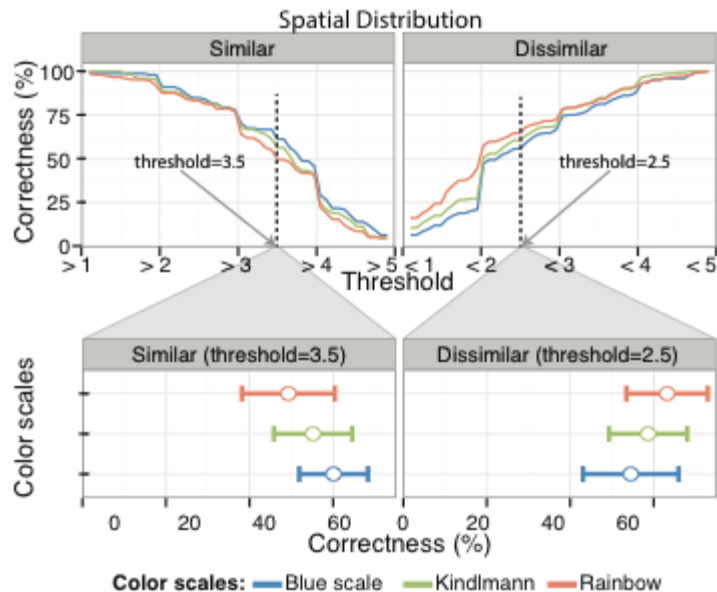
Task 1 - Magnitude Estimation

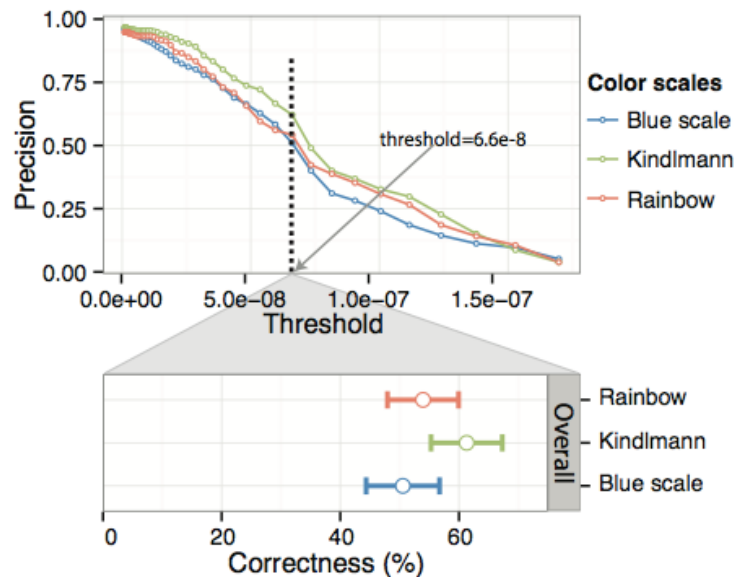Task 2 - Similarity Estimation

Task 3 - Area Identification
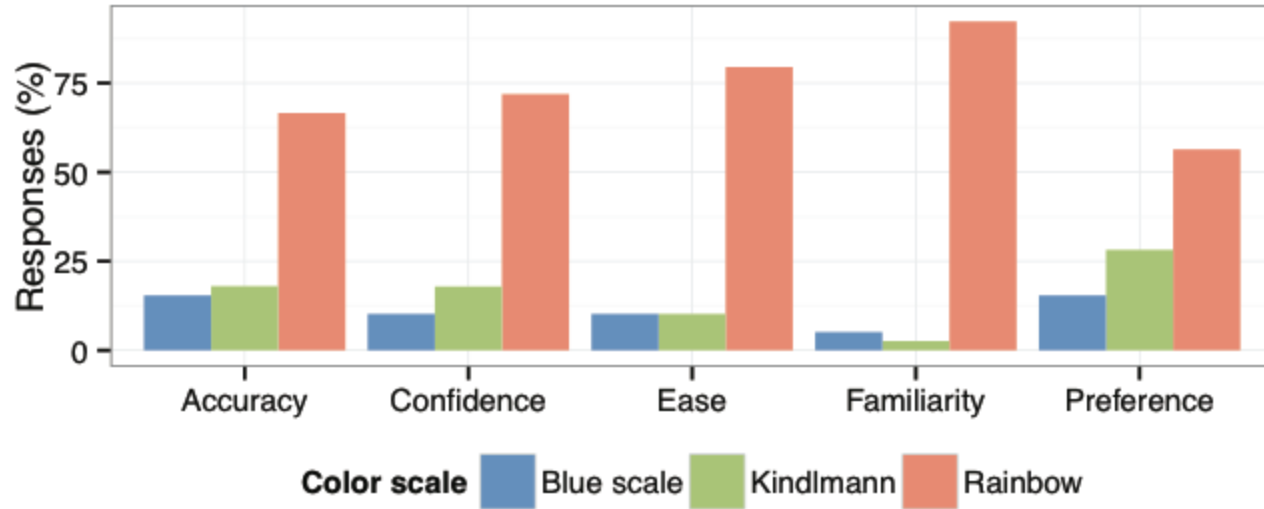
MAGNITUDE ESTIMATION

SIMILARITY ESTIMATION

AREA IDENTIFICATION
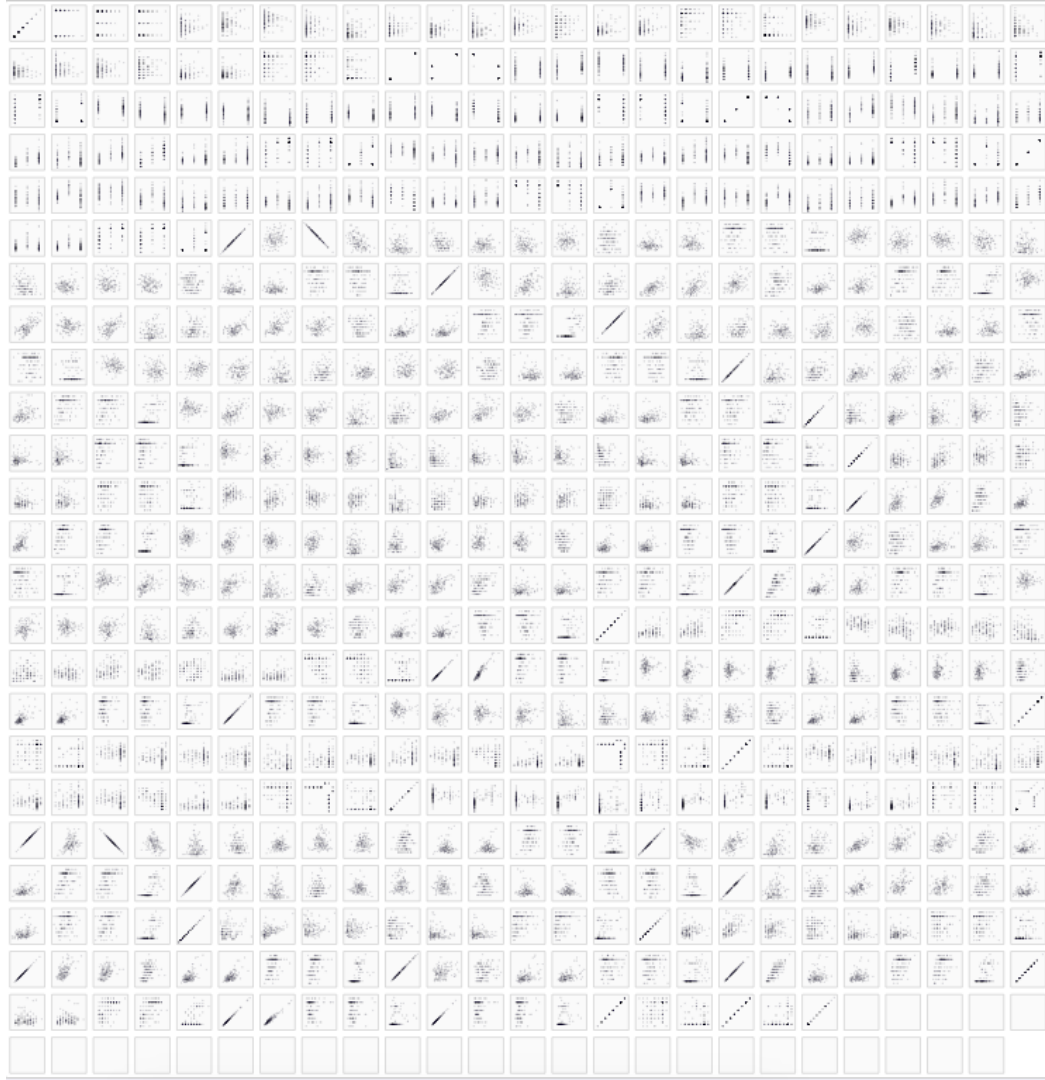
SUBJECTIVE PERCEPTION OF PERFORMANCE

Selected Challenges

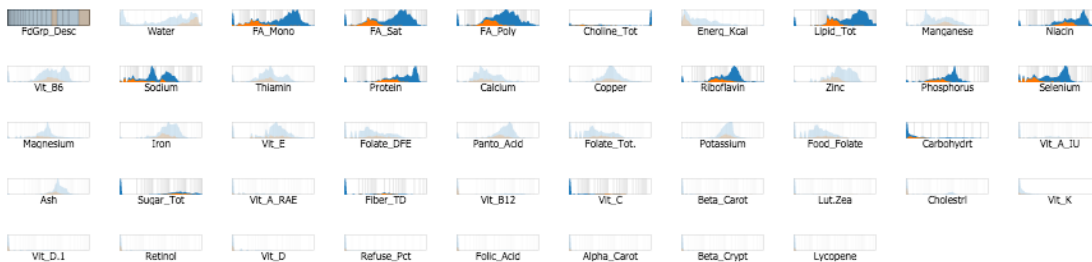Automated and Interactive Methods.

High-Dimensional Data Spaces.

Evidence-Based Guidelines for Vis Design.

Sifting through a
million plots.

Paper: How Deceptive Are Deceptive Visualizations?

by ENRICO on FEBRUARY 25, 2015

in RESEARCH

We all know by now that visualization, thanks to its amazing communication powers, can be used to communicate effectively and persuasively massages that stick into people's mind. This same power, however, can also be used to mislead and misinform people very effectively! When techniques like non-zero baselines, scaling by area (quadratic change to represent linear changes), bad color maps, etc., are used, it is very easy to communicate the *wrong* message to your readers (being that done on purpose or for lack of better knowledge). But, how easy is it?
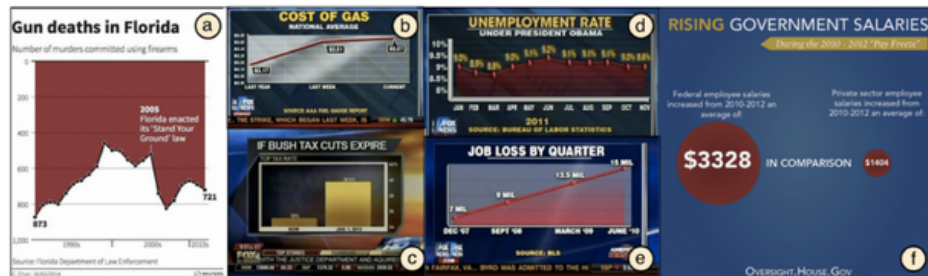
How easy is it to deceive people with visualization?

http://fellinlovewithdata.com

DATA STORIES

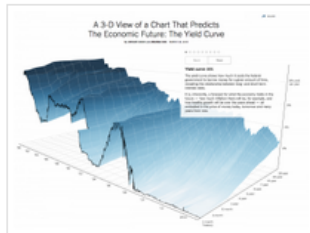A podcast on data visualization with Enrico Bertini and Moritz Stefaner

Data Stories tv#00 — The NYT 3D Yield Curve Chart w/ Gregor Aisch

MP3 Audio [0 B] | Download | Show URL

Hi Folks, great news … we are experimenting with a new format for Data Stories that includes … that includes … that includes … guess whaaaaaat? Video!

After having heard many many times that it's hard to imagine how a visualization looks like when we are talking about it, we have decided to experiment with a new format.

This is for now just a pilot to see how you guys react, so we would love to hear your feedback about how you like it and how we can improve.

To be clear: **we are not planning to substitute our regular podcast with this**, we are trying to build a parallel channel.

—

Here's the video!

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Thanks! Questions?

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